

High-Order Discontinuous Galerkin Remap Methods for Curvilinear ALE Hydrodynamics

MultiMat 2013, San Francisco

September 3, 2013

R. Anderson, V. Dobrev, Tz. Kolev,
R. Rieben and V. Tomov



We are developing high-order ALE discretization methods for large-scale hydrodynamic simulations

The Arbitrary Lagrangian-Eulerian (ALE) framework for the equations of shock hydrodynamics is the foundation of many large-scale simulation codes.

ALE Equations

Momentum Conservation: $\rho \left(\frac{d\vec{v}}{dt} + \vec{c} \cdot \nabla \vec{v} \right) = \nabla \cdot \sigma$

Mass Conservation: $\frac{d\rho}{dt} + \vec{c} \cdot \nabla \rho = -\rho \nabla \cdot \vec{v}$

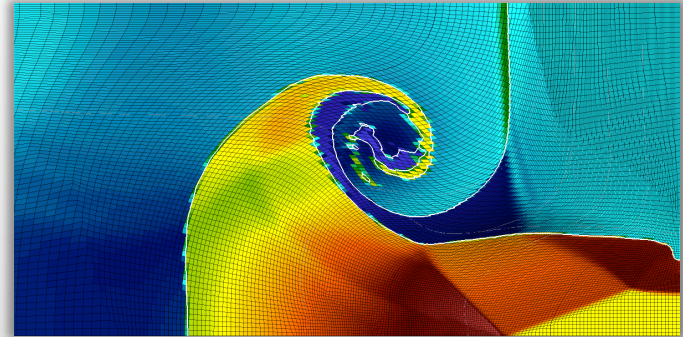
Energy Conservation: $\rho \left(\frac{de}{dt} + \vec{c} \cdot \nabla e \right) = \sigma : \nabla \vec{v}$

Equation of State: $p = EOS(e, \rho)$

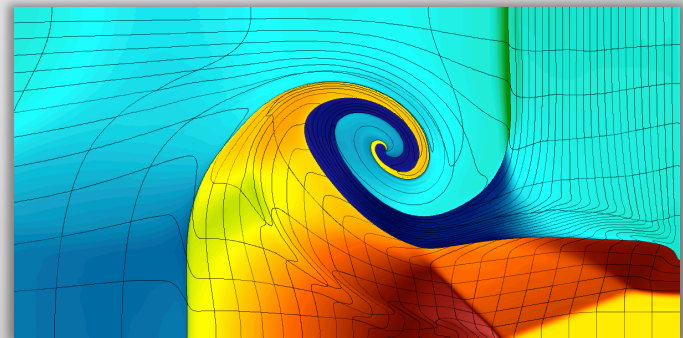
Equation of Motion: $\frac{d\vec{x}}{dt} + \vec{c} = \vec{v}$

ALE discretization approaches consist of:

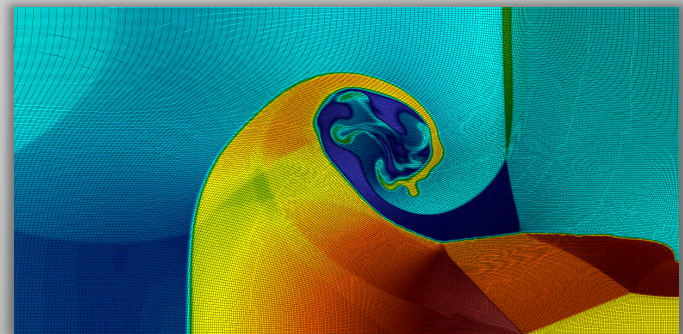
- Lagrange phase
 - mesh optimization step
 - field remap step
 - multi-material zone treatment step
- } “advection” phase



Traditional ALE simulation



High-order Lagrangian simulation



High-order ALE simulation

High-order curvilinear Lagrangian discretizations pose challenges and need a matching accurate “advection” phase

We have developed **BLAST** - a high-order research Lagrangian hydrocode featuring:

- Curvilinear mesh zones
- High-order kinematic and thermodynamic fields
- Exact conservation on semi-discrete level

Semi-discrete finite element method

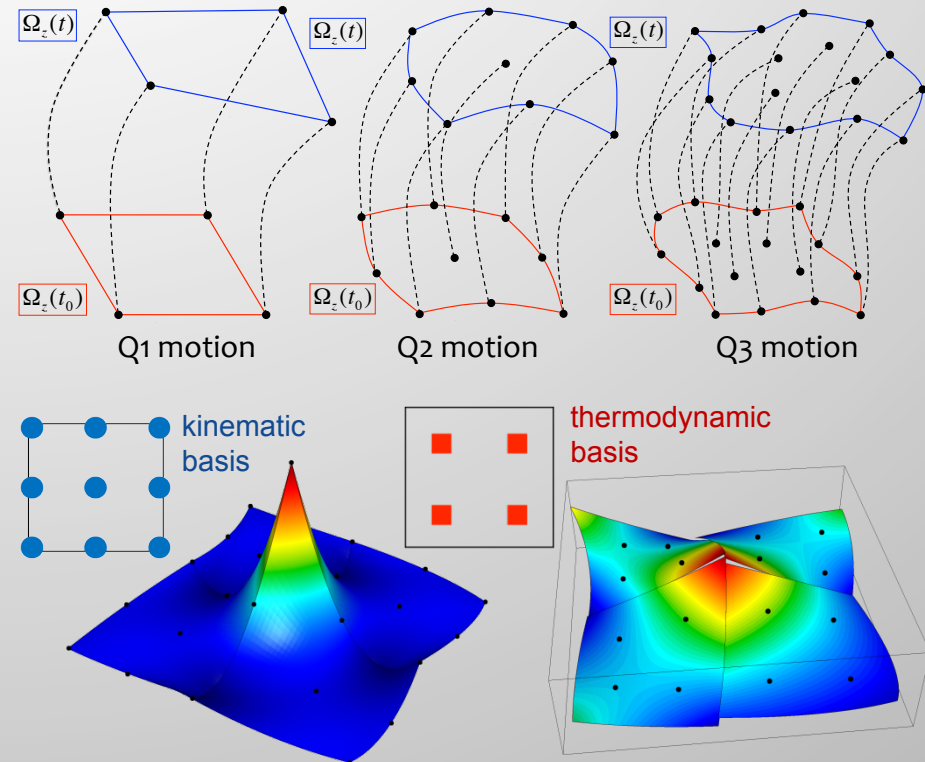
Momentum Conservation: $\mathbf{M}_v \frac{d\mathbf{v}}{dt} = -\mathbf{F} \cdot \mathbf{1}$

Energy Conservation: $\mathbf{M}_e \frac{de}{dt} = \mathbf{F}^T \cdot \mathbf{v}$

Equation of Motion: $\frac{d\mathbf{x}}{dt} = \mathbf{v}$

- FLOP-intensive numerical kernel $(\mathbf{F})_{ij} = \int_{\Omega(t)} (\sigma : \nabla \vec{w}_i) \phi_j$
- Generalizations of classical SGH schemes

- ① Kolev and Rieben, A tensor artificial viscosity using a finite element approach, *JCP*, 2009.
- ② Dobrev, Ellis, Kolev and Rieben, Curvilinear finite elements for Lagrangian hydrodynamics, *IJNMF*, 2010.
- ③ Dobrev, Kolev and Rieben, High order curvilinear finite element methods for Lagrangian hydrodynamics, *SISC*, 2012.
- ④ Dobrev, Ellis, Kolev and Rieben, High order curvilinear finite elements for axisymmetric Lagrangian hydrodynamics, *CAF*, 2012.
- ⑤ Dobrev, Kolev and Rieben, High order curvilinear finite elements for elastic-plastic Lagrangian dynamics, *JCP*, 2013.
- ⑥ **BLAST**: High-order curvilinear finite element code for Lagrangian shock hydrodynamics, <http://www.llnl.gov/casc/blast>
- ⑦ **MFEM**: Parallel finite element discretization library, <http://mfem.googlecode.com>



We have developed high-order extensions of classical linear and nonlinear mesh optimization algorithms

Harmonic mesh smoothing can be written in terms of a **mesh Laplacian** and a **smoother** as a simple linear iteration:

$$\mathbf{x}^{n+1} = \mathbf{x}^n + M^{-1}(f - L\mathbf{x}^n)$$

The smoother can be used for spectral filtering.

In general, harmonic smoothing is an **integral minimization problem** with an **energy function**:

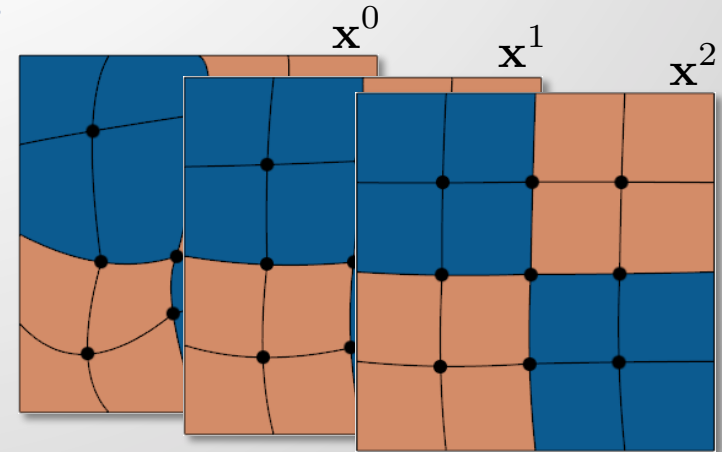
$$\min_{\mathbf{x}_I} \left(\frac{1}{2} \sum_E \int_{\hat{E}} \nabla \Phi_E : \nabla \Phi_E \right) = \min_{\mathbf{x}_I} \sum_E \int_{\hat{E}} W(J_E(\hat{x})) d\hat{x} \longrightarrow W(J) \equiv \frac{1}{2} (J : J) = \frac{1}{2} \text{tr}(J^T J)$$

The **inverse-harmonic** (Winslow-Crowley) method can be written as:

$$\min_{\mathbf{x}_I} \left(\frac{1}{2} \sum_E \int_E \nabla(\Phi_E^{-1}) : \nabla(\Phi_E^{-1}) \right) = \min_{\mathbf{x}_I} \sum_E \int_{\hat{E}} W(J_E(\hat{x})) d\hat{x} \longrightarrow W(J) \equiv \frac{1}{2} \det(J) \text{tr}(J^{-T} J^{-1})$$

The **general non-linear smoothing** method can be written for any energy function as:

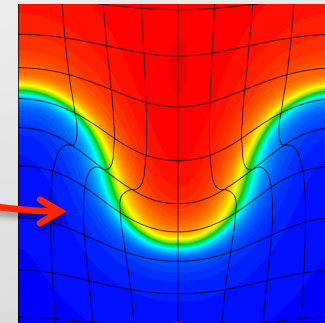
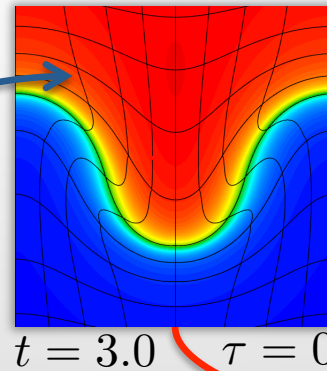
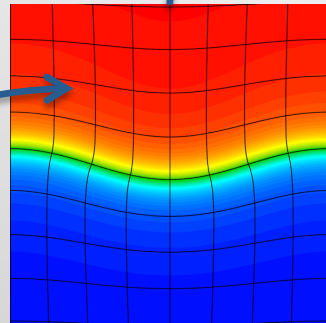
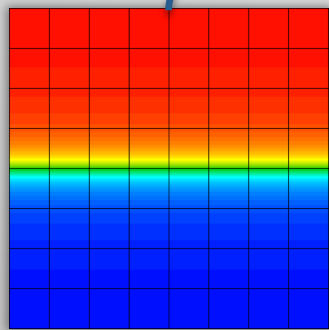
$$\mathbf{x}^{n+1} = \mathbf{x}^n - [\mathcal{H}F(\mathbf{x}^n)]^{-1} \nabla F(\mathbf{x}^n)$$



We have developed high-order “pseudo-time” DG advection algorithms for conservative and accurate remap

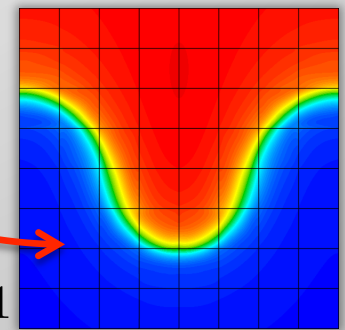
Lagrangian phase

- ❖ mesh motion determined by physical velocity
- ❖ time t evolution



Advection phase

- ❖ artificial mesh motion, defining the mesh velocity
- ❖ “pseudo-time” τ evolution



Both phases

- ✓ material derivative based on particle trajectories

$$\frac{d\rho}{dt} \equiv \frac{\partial \rho}{\partial t} + v_m \cdot \nabla \rho$$

- ✓ Deforming test functions

$$\frac{d\psi}{dt} = 0$$

- ✓ Reynolds transport theorem

$$\frac{\partial}{\partial t} \int_{U(t)} \rho = \int_{U(t)} \frac{d\rho}{dt} + \rho \nabla \cdot v_m$$

Lagrangian phase ($\vec{c} = \vec{0}$)

Momentum Conservation: $\rho \frac{d\vec{v}}{dt} = \nabla \cdot \sigma$

Mass Conservation: $\frac{d\rho}{dt} = -\rho \nabla \cdot \vec{v}$

Energy Conservation: $\rho \frac{de}{dt} = \sigma : \nabla \vec{v}$

Equation of Motion: $\frac{d\vec{x}}{dt} = \vec{v}$

Advection phase ($\vec{c} = -\vec{v}_m$)

Momentum Conservation: $\frac{d(\rho \vec{v})}{d\tau} = \vec{v}_m \cdot \nabla (\rho \vec{v})$

Mass Conservation: $\frac{d\rho}{d\tau} = \vec{v}_m \cdot \nabla \rho$

Energy Conservation: $\frac{d(\rho e)}{d\tau} = \vec{v}_m \cdot \nabla (\rho e)$

Mesh velocity: $\vec{v}_m = \frac{d\vec{x}}{d\tau}$

Discontinuous Galerkin weak formulation of pseudo-time advection of discontinuous fields

Element-wise weak formulation of **pseudo-time advection** based on:
linear motion ($v_m = u$), pseudo-time RTT and deforming test functions

$$\boxed{\frac{d\rho}{d\tau} = u \cdot \nabla \rho}$$

$$\begin{aligned} \frac{\partial}{\partial \tau} \int_{\Omega} \rho \psi &= \int_{\Omega} \frac{d}{d\tau} (\rho \psi) + \rho \psi \nabla \cdot u = \int_{\Omega} u \cdot \nabla \rho \psi + \rho \psi \nabla \cdot u = \int_{\Omega} \nabla \cdot (\rho u) \psi \\ &= \sum_{T \in \mathcal{T}(\tau)} \int_T \nabla \cdot (\rho u) \psi = - \sum_{T \in \mathcal{T}(\tau)} \int_T \rho u \cdot \nabla \psi + \int_{\partial T} \rho u \cdot n \psi \\ &= - \sum_{T \in \mathcal{T}(\tau)} \int_T \rho u \cdot \nabla \psi + \sum_{f \in \mathcal{F}_i(\tau)} \int_f \{ \rho(u \cdot n_f) \} [\![\psi]\!] + \sum_{f \in \mathcal{F}_b(\tau)} \int_f \{ \rho(u \cdot n_f) \} [\![\psi]\!] \end{aligned}$$

Discontinuous Galerkin method with Godunov (upwind) flux $\{ \rho(u \cdot n_f) \}_* = \rho_u(u \cdot n_f)$

$$\frac{\partial}{\partial \tau} \int_{\Omega} \rho \psi = - \sum_{T \in \mathcal{T}(\tau)} \int_T \rho u \cdot \nabla \psi + \sum_{f \in \mathcal{F}_i(\tau)} \int_f (u \cdot n_f) \{ \rho \} [\![\psi]\!] - \frac{1}{2} \sum_{f \in \mathcal{F}_i(\tau)} \int_f |u \cdot n_f| [\![\rho]\!] [\![\psi]\!]$$

Matrix form assuming trial and test function in the same FEM space with mass matrix \mathbf{M} :

$$\boxed{\frac{\partial}{\partial \tau} (\mathbf{M} \boldsymbol{\rho}) = \mathbf{A} \boldsymbol{\rho}}$$

Properties: $\mathbf{A}^T \mathbf{1} = 0$, $\mathbf{S} = \mathbf{S}^T$, $\mathbf{S} \mathbf{1} = 0$

$$\frac{\partial \mathbf{M}}{\partial \tau} = (\mathbf{A} + \mathbf{S}) + (\mathbf{A} + \mathbf{S})^T$$

High-order DG advection algorithms for conservative and accurate remap

moment-based
formulation

$$\frac{\partial \mathbf{m}}{\partial \tau} = \mathbf{A} \mathbf{M}^{-1} \mathbf{m} \quad m(\tau) \equiv \int_{\Omega(\tau)} \rho \psi = \mathbf{M} \rho$$

→ mass conservation: $\frac{\partial}{\partial \tau} (\mathbf{1}^T \mathbf{m}) = \mathbf{1}^T \frac{\partial \mathbf{m}}{\partial \tau} = (\mathbf{1}^T \mathbf{A}) \mathbf{M}^{-1} \mathbf{m} = 0$

function-based
formulation

$$\frac{\partial \rho}{\partial \tau} = -\mathbf{M}^{-1} (\mathbf{A}^T + 2\mathbf{S}) \rho$$

→ preservation of constants, linears: $\frac{\partial \mathbf{1}}{\partial \tau} = -\mathbf{M}^{-1} (\mathbf{A}^T + 2\mathbf{S}) \mathbf{1} = 0$

- Finite element functions are remapped by integrating the above ODEs in pseudo-time.
- The two approaches are the same on semi-discrete but differ on fully-discrete level.
- Mass conservation + constant preservation can be achieved on fully-discrete level by integrating the mass matrix in pseudo-time.
- A space-time DG method related to these approaches can be viewed as high-order generalization of the classical “swept-volume” method.

To ensure monotonicity for discontinuous fields, we have adapted ideas from the FCT community

function-based
formulation

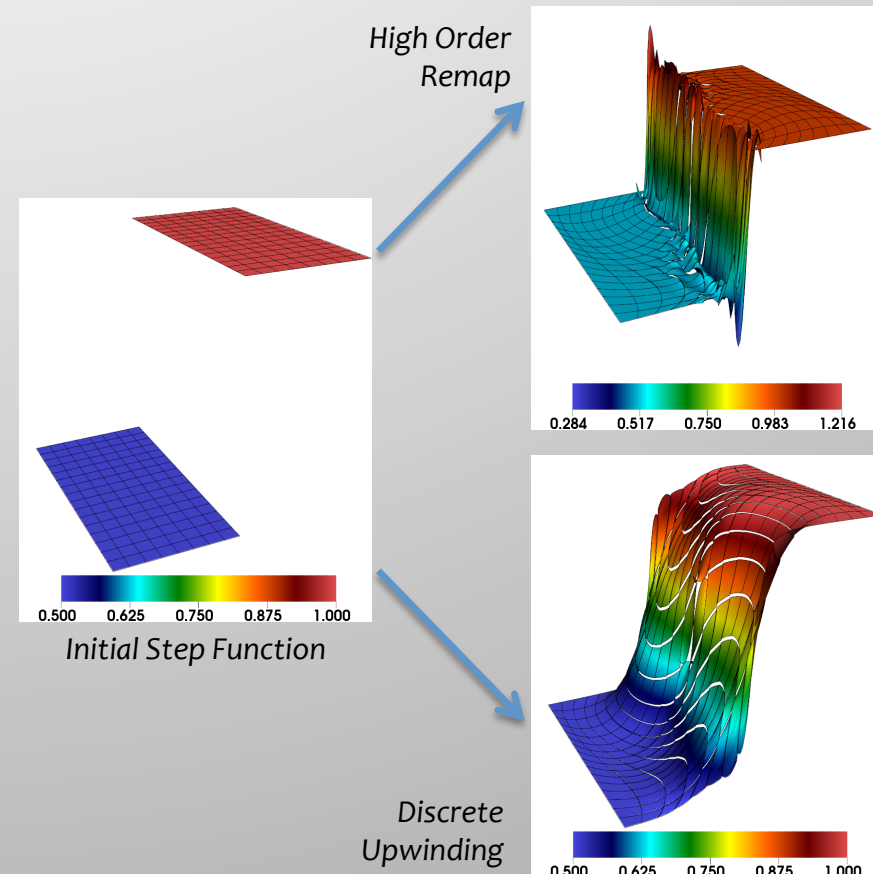
$$\sum_j \mathbf{M}_{ij} \frac{\partial \rho_j}{\partial \tau} = \sum_{j \neq i} \mathbf{K}_{ij} (\rho_i - \rho_j) \quad \text{where} \quad \mathbf{K} = -(\mathbf{A}^T + 2\mathbf{S})$$

- Monotonicity is **guaranteed** by lumping the mass matrix and enforcing:

$$\frac{\partial \rho_i}{\partial \tau} = \frac{1}{m_i} \sum_{j \neq i} \mathbf{K}_{ij} (\rho_i - \rho_j)$$

$$\mathbf{K}_{ij} \geq 0, \quad \forall j \neq i$$

- Discrete **upwinding** yields a monotonic **1st order accurate** solution
- Several high-order approaches:
 - ✓ **Locally-scaled upwind diffusion (LSD)**
 - ✓ **High-order FCT (Kuzmin)**
 - ✓ **High-order OBR (Rizdal, Bochev)**



Locally scaled upwind diffusion is used to partially lump/upwind the matrices based on the current solution

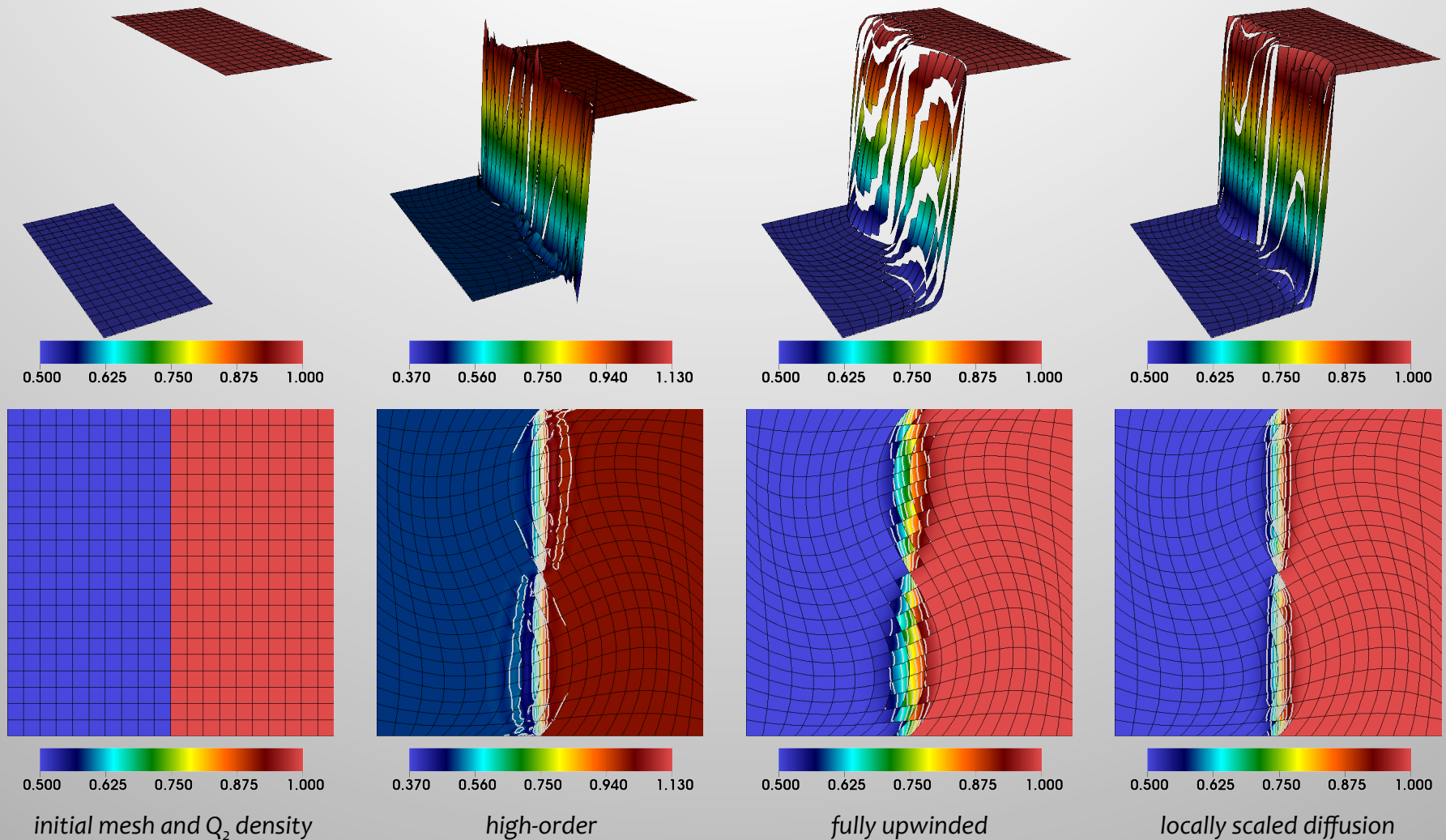
- Unlike FCT, we start with the high-order solution on fully-discrete level, and locally upwind/lump to ensure monotonicity
- **Monotonicity coefficient** measures the deviation from previous min/max values in a **neighborhood** after each time step:
$$\mu(\rho_i) = \begin{cases} 1, & \text{if } \rho_i > \rho_i^{max} \\ 1, & \text{if } \rho_i < \rho_i^{min} \\ 0 & \text{otherwise} \end{cases}$$
- The off-diagonals of the mass and advection matrices are modified after each locally scaled upwind diffusion iteration (diagonals are modified to preserve rowsums)

$$\mathbf{M}_{ij} \mapsto \mathbf{M}_{ij} - \mu_{ij} \mathbf{M}_{ij} , \quad \mathbf{K}_{ij} \mapsto \mathbf{K}_{ij} - \mu_{ij} \min\{0, \mathbf{K}_{ij}, \mathbf{K}_{ji}\}$$

with the symmetric monotonicity scaling factor $\mu_{ij} = \max(\mu(\rho_i), \mu(\rho_j))$

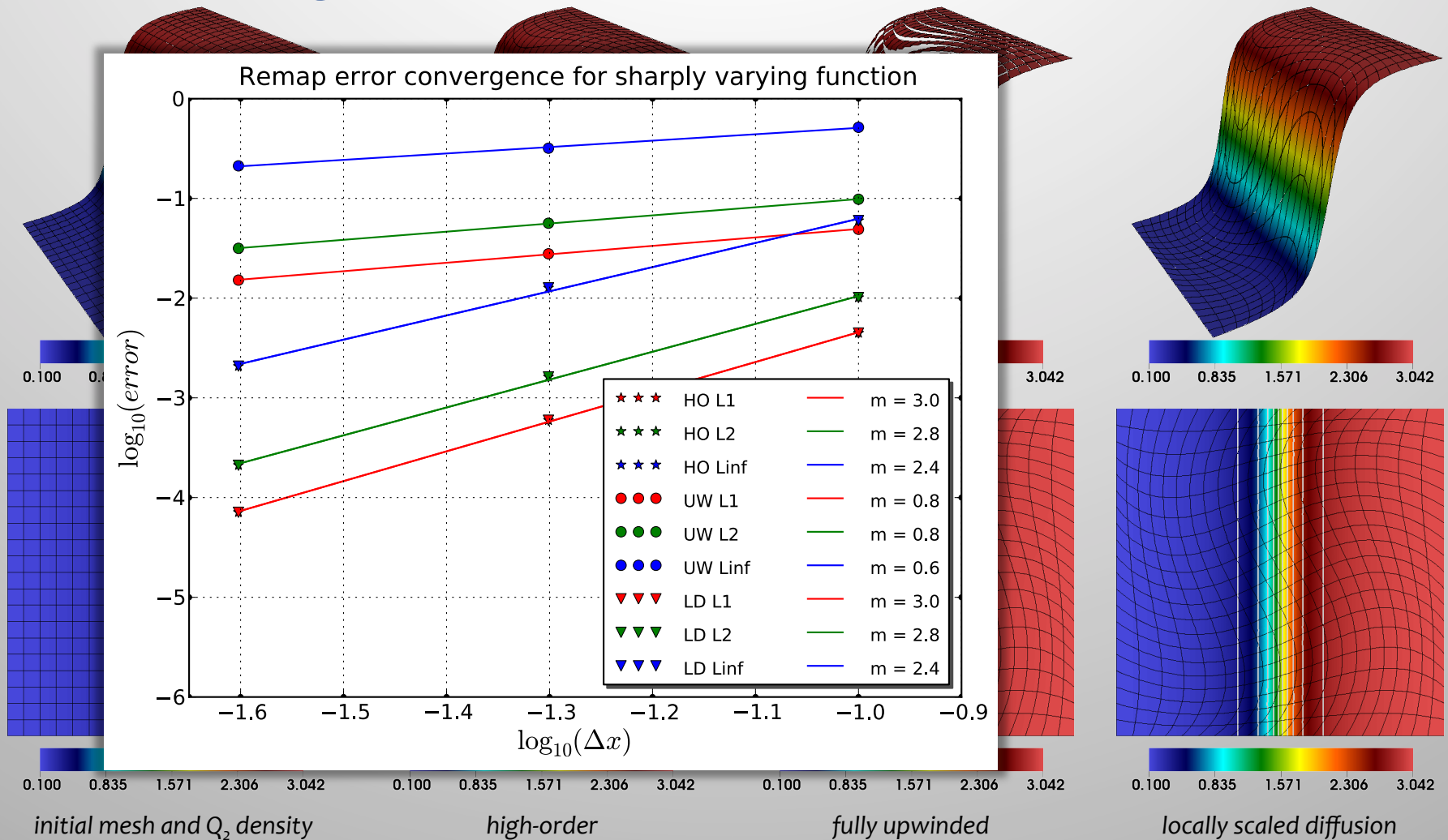
- The local diffusion coefficient is used to locally lump / upwind the matrices in an **iterative process**:
 1. Begin with zero value of monotonicity coefficient
 2. Perform locally scaled remap step and compute **monotonicity metric**
 3. If metric is non-zero, update monotonicity coefficient and **return to step 2**, else exit

Remapping results using Locally Scaled Upwind Diffusion for a discontinuous density field



Remap based on Q_2 Bernstein density and 100 steps of RK2. *The remapped function is monotonic!*

Remapping results using Locally Scaled Upwind Diffusion for a sharply varying density field



Remap based on Q_2 Bernstein density and 100 steps of RK2. *High-order approximation is recovered!*

Multi-field ALE remap is formulated as a general system of ODEs in pseudo-time

The **ALE remap step in BLAST** solves the coupled function-based advection equations as a system of ODEs using high-order explicit time integrators (e.g. RK4)

$$\boxed{\frac{\partial Y}{\partial \tau} = \mathcal{F}(Y, \tau)} \quad \text{where } Y = (\rho, \mathbf{v}, \mathbf{e}) \quad \text{and} \quad \mathcal{F}(Y, \tau) = \begin{pmatrix} \mathbf{M}_\rho^{-1} \mathbf{K}_\rho \rho \\ \mathbf{M}_\mathbf{v}^{-1} \mathbf{K}_\mathbf{v} \mathbf{v} \\ \mathbf{M}_\mathbf{e}^{-1} \mathbf{K}_\mathbf{e} \mathbf{e} \end{pmatrix}$$

Density remap pseudo-time advection of *mass* using *discontinuous* FEM space

$$\frac{d\rho}{d\tau} = u \cdot \nabla \rho \quad \mapsto \quad \frac{\partial}{\partial \tau} \int_{\Omega} \rho \psi = - \sum_T \int_T \rho u \cdot \nabla \psi + \sum_f \int_f \rho_u (u \cdot n_f) \llbracket \psi \rrbracket$$

Function-based density remap: $\mathbf{M}_\rho \frac{\partial \rho}{\partial \tau} = \mathbf{K}_\rho \rho$, where $\mathbf{K}_\rho = -(\mathbf{A}_\rho^T + 2\mathbf{S}_\rho)$.

- $\mathbf{K}_\rho \mathbf{1} = 0$ \rightarrow preservation of constants
- $\mathbf{K}_\rho^T \mathbf{1} = -\frac{\partial \mathbf{M}_\rho}{\partial \tau} \mathbf{1}$ \rightarrow conservation of mass
- $\frac{\partial \mathbf{M}_\rho}{\partial \tau} = \mathbf{A}_\rho - \mathbf{K}_\rho$ \rightarrow equivalence with moment-based remap

Multi-field ALE remap is formulated as a general system of ODEs in pseudo-time

The **ALE remap step in BLAST** solves the coupled function-based advection equations as a system of ODEs using high-order explicit time integrators (e.g. RK4)

$$\boxed{\frac{\partial Y}{\partial \tau} = \mathcal{F}(Y, \tau)} \quad \text{where } Y = (\rho, \mathbf{v}, \mathbf{e}) \quad \text{and} \quad \mathcal{F}(Y, \tau) = \begin{pmatrix} \mathbf{M}_\rho^{-1} \mathbf{K}_\rho \rho \\ \mathbf{M}_\mathbf{v}^{-1} \mathbf{K}_\mathbf{v} \mathbf{v} \\ \mathbf{M}_\mathbf{e}^{-1} \mathbf{K}_\mathbf{e} \mathbf{e} \end{pmatrix}$$

IE remap advection of *internal energy* using *discontinuous* FEM space

$$\frac{d(\rho e)}{d\tau} = u \cdot \nabla(\rho e) \quad \mapsto \quad \frac{\partial}{\partial \tau} \int_\Omega \rho(e\psi) = - \sum_T \int_T \rho(eu \cdot \nabla \psi) + \sum_f \int_f \rho_u(u \cdot n_f) \{e\} \llbracket \psi \rrbracket - \frac{1}{2} \rho_u |u \cdot n_f| \llbracket e \rrbracket \llbracket \psi \rrbracket$$

Function-based energy remap: $\mathbf{M}_\mathbf{e} \frac{\partial \mathbf{e}}{\partial \tau} = \mathbf{K}_\mathbf{e} \mathbf{e}$, where $\mathbf{K}_\mathbf{e} = -(\mathbf{A}_\mathbf{e}^T + 2\mathbf{S}_\mathbf{e})$.

- $\mathbf{K}_\mathbf{e} \mathbf{1} = 0$ \rightarrow preservation of constants
- $\mathbf{K}_\mathbf{e}^T \mathbf{1} = -\frac{\partial \mathbf{M}_\mathbf{e}}{\partial \tau} \mathbf{1}$ \rightarrow conservation of internal energy if $Q_\mathbf{e} \subseteq Q_\rho$
- $\frac{\partial \mathbf{M}_\mathbf{e}}{\partial \tau} = \mathbf{A}_\mathbf{e} - \mathbf{K}_\mathbf{e}$ \rightarrow equivalence with moment-based remap if $Q_\mathbf{e}^2 \subseteq Q_\rho$

Multi-field ALE remap is formulated as a general system of ODEs in pseudo-time

The **ALE remap step in BLAST** solves the coupled function-based advection equations as a system of ODEs using high-order explicit time integrators (e.g. RK4)

$$\boxed{\frac{\partial Y}{\partial \tau} = \mathcal{F}(Y, \tau)} \quad \text{where } Y = (\rho, \mathbf{v}, \mathbf{e}) \quad \text{and} \quad \mathcal{F}(Y, \tau) = \begin{pmatrix} \mathbf{M}_\rho^{-1} \mathbf{K}_\rho \rho \\ \mathbf{M}_\mathbf{v}^{-1} \mathbf{K}_\mathbf{v} \mathbf{v} \\ \mathbf{M}_\mathbf{e}^{-1} \mathbf{K}_\mathbf{e} \mathbf{e} \end{pmatrix}$$

Velocity remap pseudo-time advection of **momentum** using **continuous** FEM space

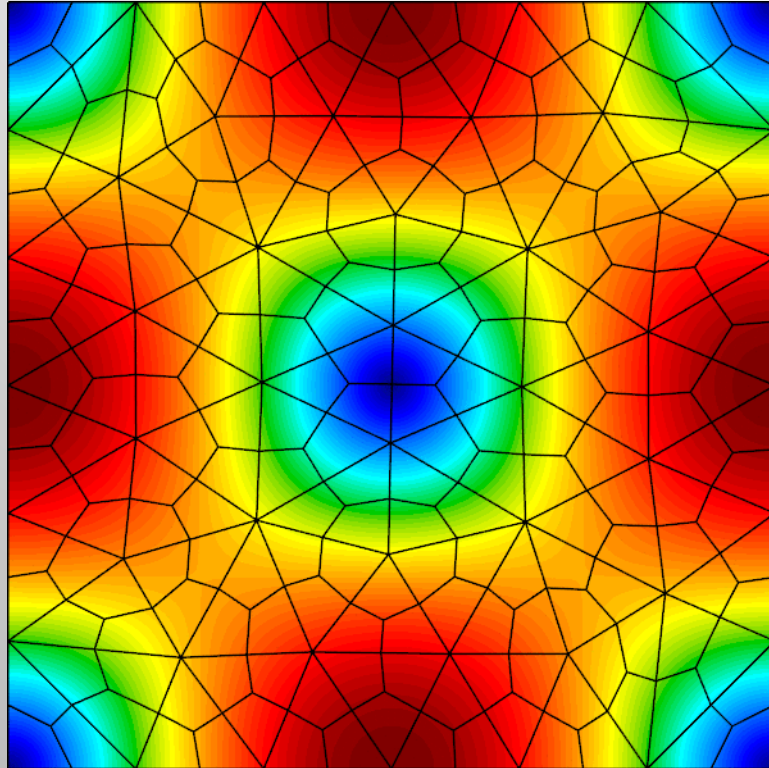
$$\frac{d(\rho v)}{d\tau} = u \cdot \nabla(\rho v) \quad \mapsto \quad \frac{\partial}{\partial \tau} \int_{\Omega} \rho(v \cdot w) = - \int_{\Omega} \rho(u \cdot \nabla w \cdot v)$$

Function-based velocity remap: $\mathbf{M}_\mathbf{v} \frac{\partial \mathbf{v}}{\partial \tau} = \mathbf{K}_\mathbf{v} \mathbf{v}$, where $\mathbf{K}_\mathbf{v} = -\mathbf{A}_\mathbf{v}^T$.

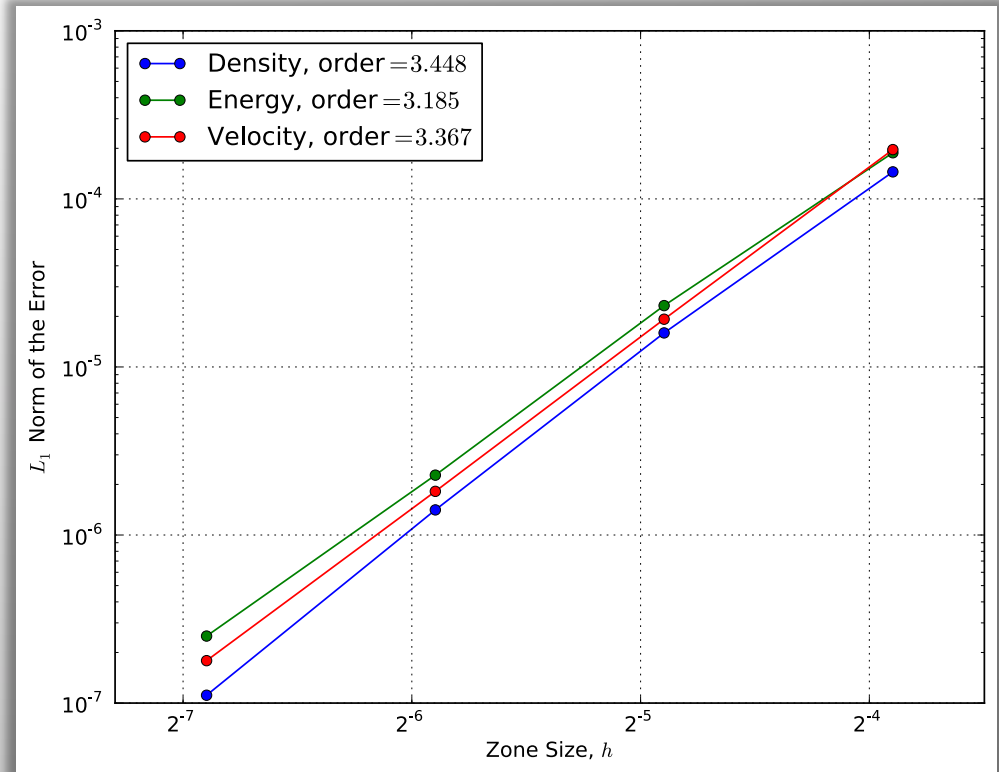
- $\mathbf{K}_\mathbf{v} \mathbf{1} = 0 \rightarrow$ preservation of constants
- $\mathbf{K}_\mathbf{v}^T \mathbf{1} = -\frac{\partial \mathbf{M}_\mathbf{v}}{\partial \tau} \mathbf{1} \rightarrow$ conservation of momentum if $Q_\mathbf{v} \subseteq Q_\rho$
- $\frac{\partial \mathbf{M}_\mathbf{v}}{\partial \tau} = \mathbf{A}_\mathbf{v} - \mathbf{K}_\mathbf{v} \rightarrow$ conservation of kinetic energy if $Q_\mathbf{v}^2 \subseteq Q_\rho$

$$\frac{\partial}{\partial \tau} \left(\frac{\mathbf{v}^T \mathbf{M}_\mathbf{v} \mathbf{v}}{2} \right) = \mathbf{v}^T \mathbf{M}_\mathbf{v} \frac{\partial \mathbf{v}}{\partial \tau} + \frac{1}{2} \mathbf{v}^T \frac{\partial \mathbf{M}_\mathbf{v}}{\partial \tau} \mathbf{v} = -\mathbf{v}^T \mathbf{A}_\mathbf{v}^T \mathbf{v} + \frac{1}{2} \mathbf{v}^T (\mathbf{A}_\mathbf{v} + \mathbf{A}_\mathbf{v}^T) \mathbf{v} = 0$$

High-order 2D Taylor-Green vortex ALE results in BLAST



Speed, up to $t=0.537$ (10 remaps)



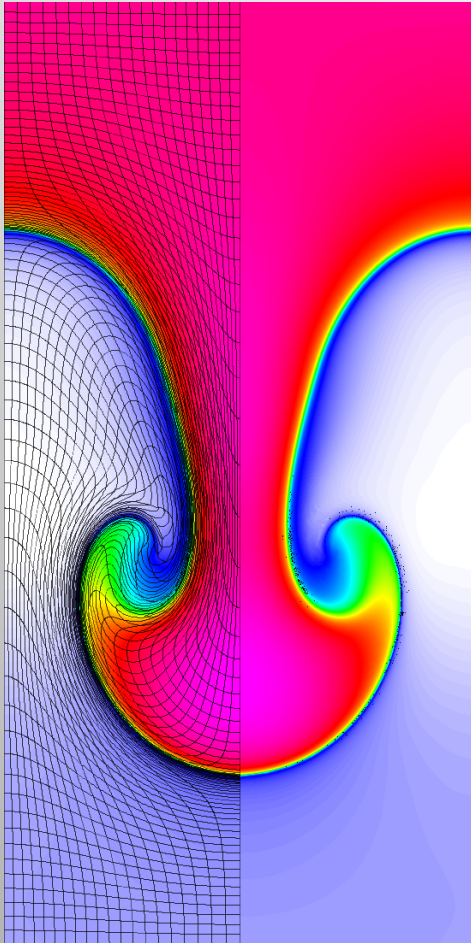
L_1 errors at $t=4.0$

Q_3 - Q_2 RK3SSP Lagrangian scheme, no artificial viscosity. “Eulerian” remap (to the initial mesh) of density, velocity and energy every 20 cycles using 6 RK3SSP steps.

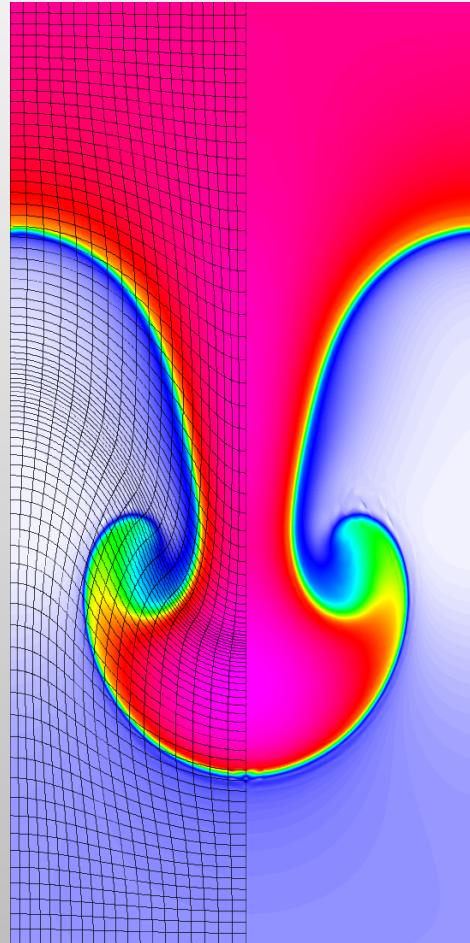
The overall ALE scheme preserves the high-order convergence!

Comparing Lagrangian, Eulerian and ALE results in BLAST for the 2D Rayleigh-Taylor problem

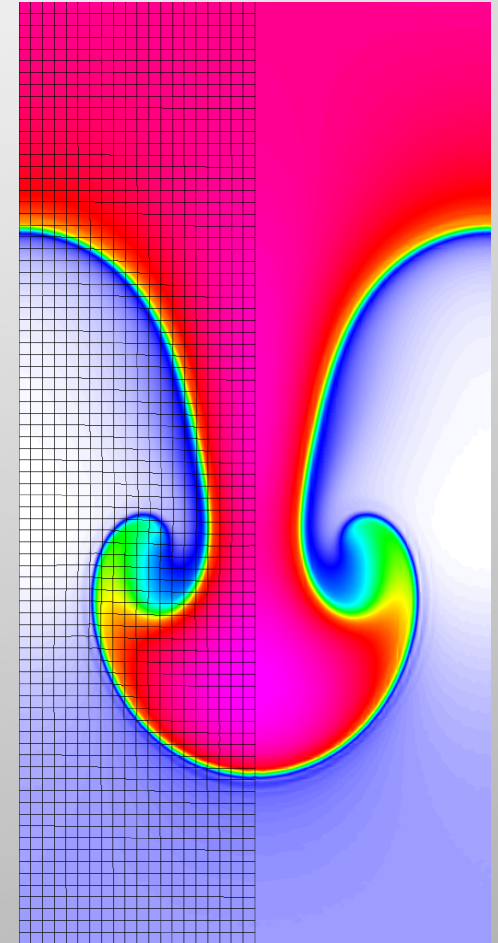
Q_4 - Q_3 RK4 Lagrangian scheme, no artificial viscosity, time $t = 4.5$



Lagrangian



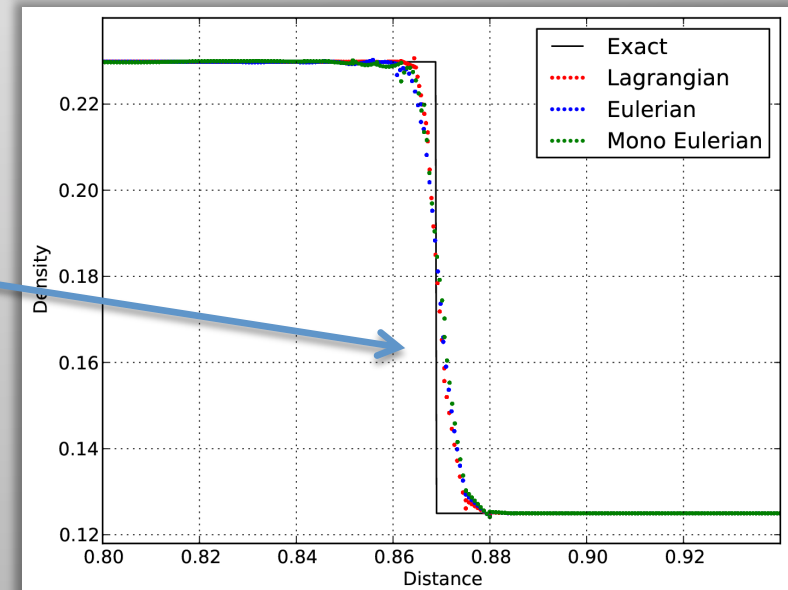
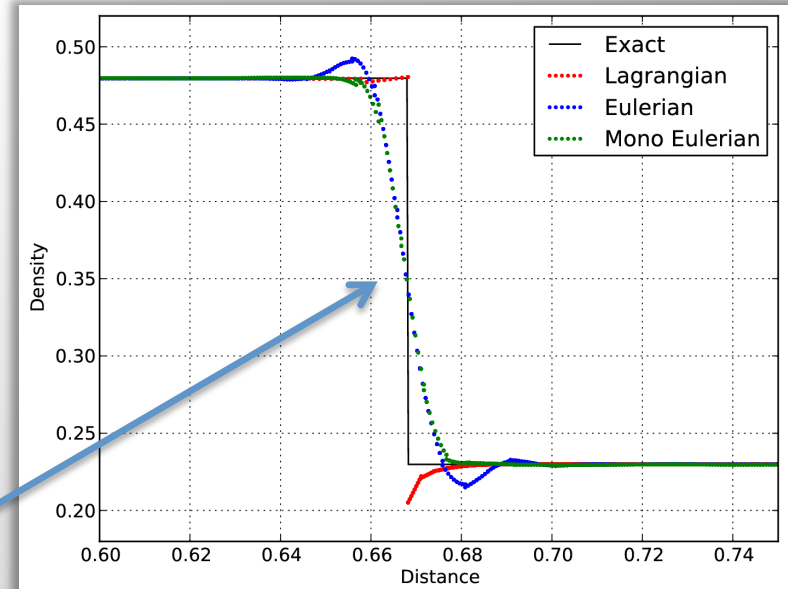
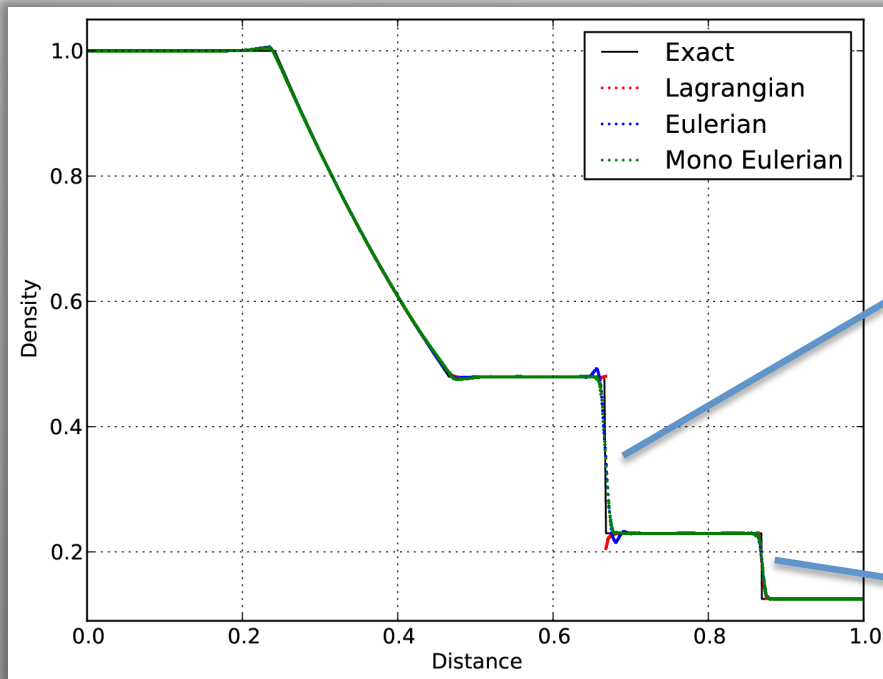
ALE (remap period = 10)
1 mesh relax iter. + 2 adv. steps/remap



Eulerian (remap period = 10)
2 adv. steps/remap

1D Sod shock tube in BLAST

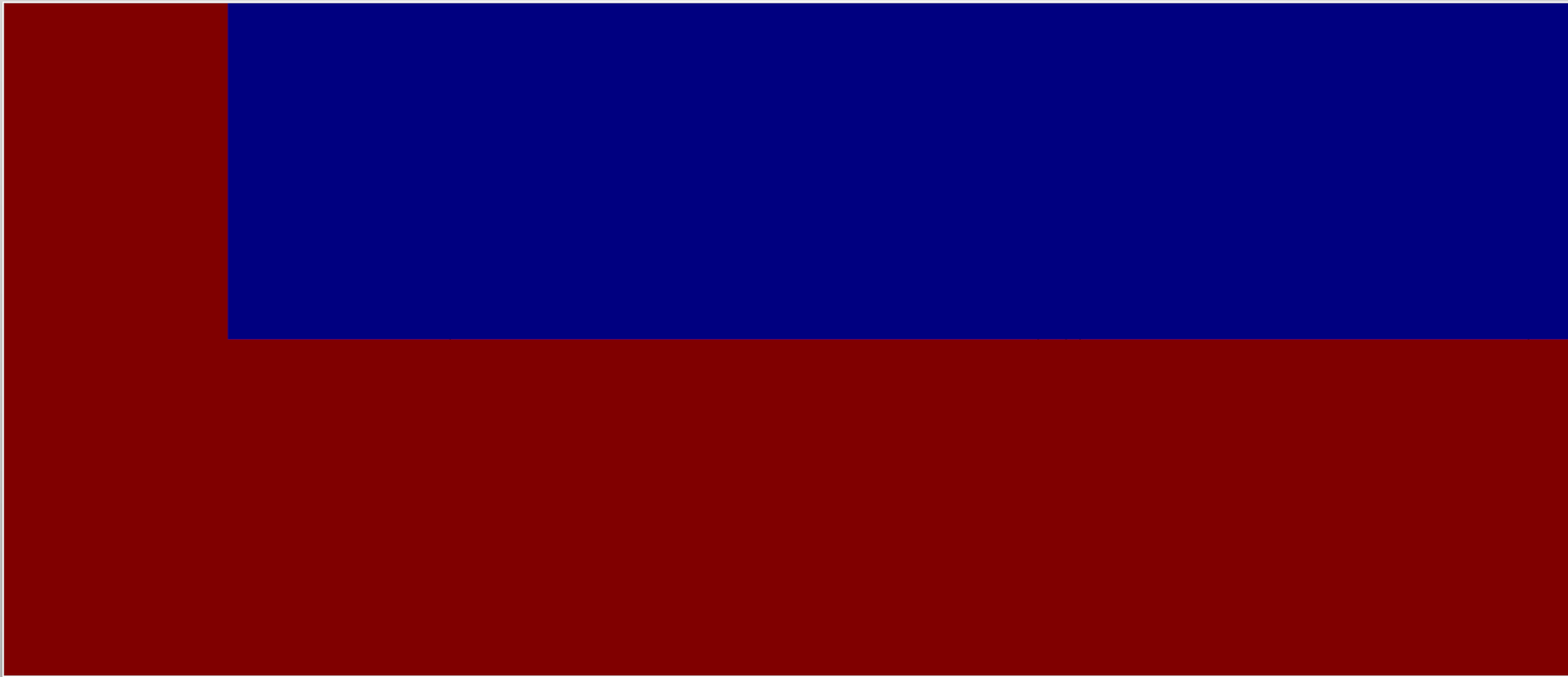
- Q_2 - Q_1 RK2Avg with artificial viscosity
- Evaluate **LSD monotonicity** treatment



Oscillations at material interface are removed, while values at the shock are not affected!

Triple-point – shock interaction ALE results in BLAST

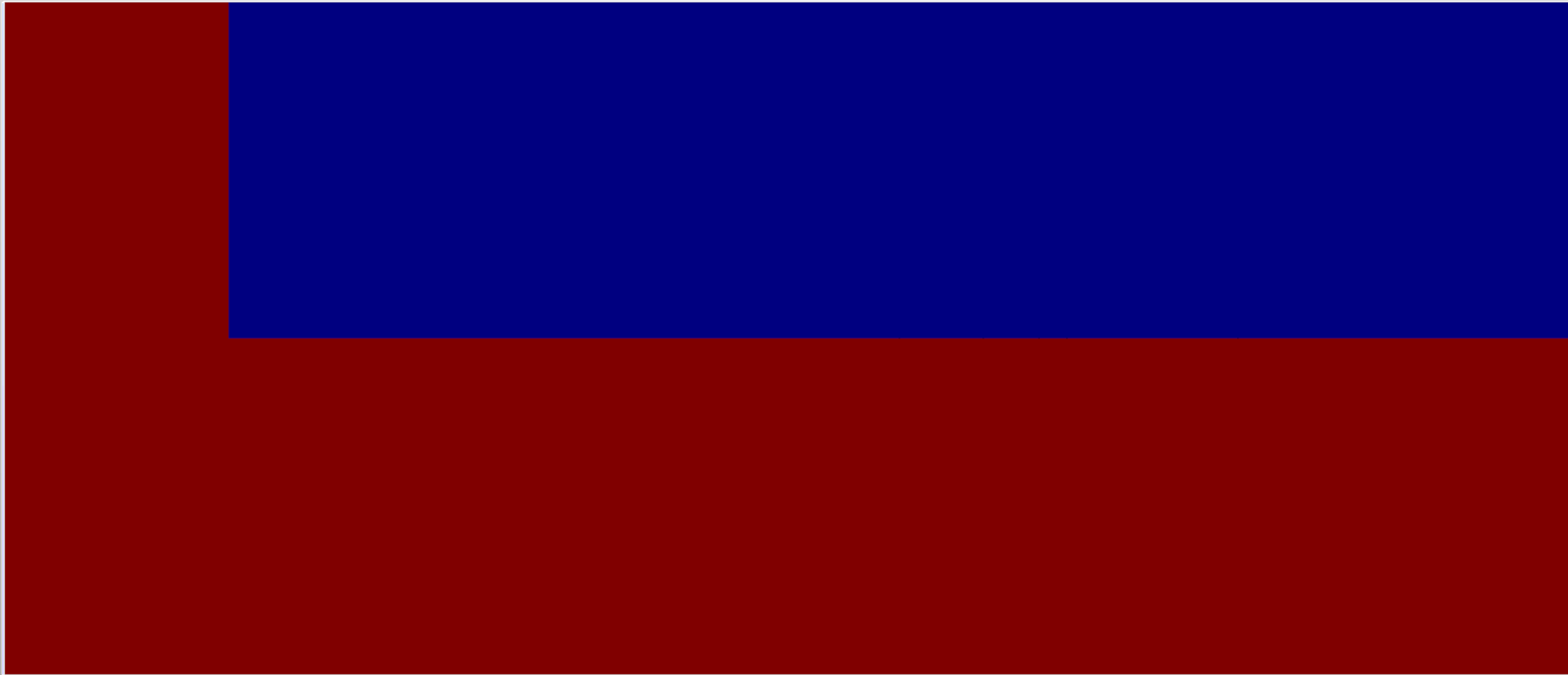
- Q_2 - Q_1 RK2Avg with hyperviscosity, 256 processors
- Periodic ALE with LSD monotonicity, Q_2 density, and adaptive pseudotime step, $t = 5$



ALE enables us to run the problem much faster than in Lagrangian mode!

Triple-point – shock interaction ALE results in BLAST

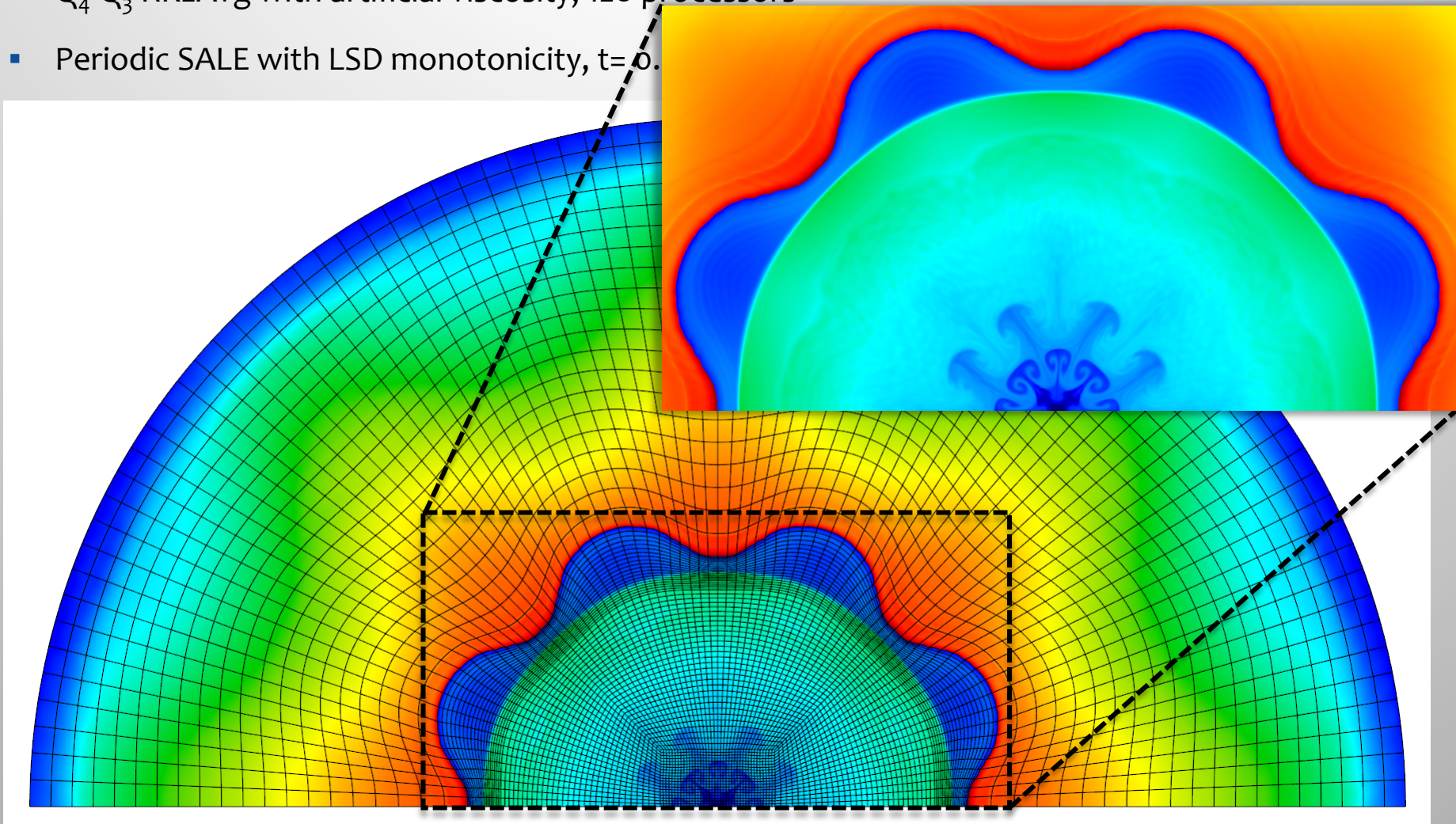
- Q_4 - Q_3 RK4 with full anisotropic tensor artificial viscosity, 512 processors
- Eulerian ALE with no monotonicity and RK4 integrator, $t = 5$



ALE enables us to run the problem much faster than in Lagrangian mode!

Perturbed ICF-like problem: SALE simulation in BLAST

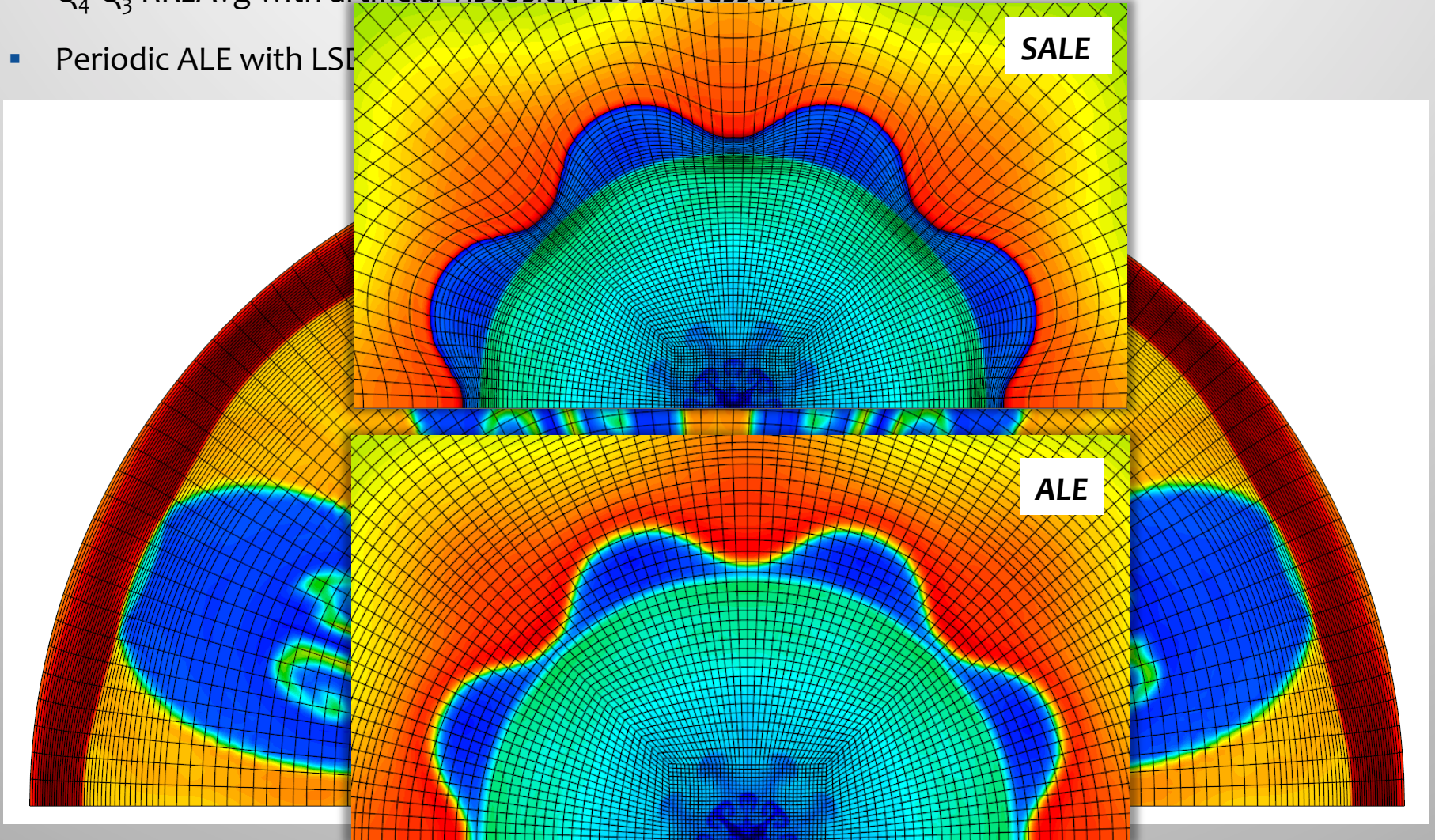
- Q_4 - Q_3 RK2Avg with artificial viscosity, 128 processors
- Periodic SALE with LSD monotonicity, $t=0$.



SALE keeps a sharp interface, but time-stepping restrictions are not completely alleviated

Perturbed ICF-like problem: ALE simulation in BLAST

- Q_4 - Q_3 RK2Avg with artificial viscosity, 128 processors
- Periodic ALE with LSI



ALE enables us to run the problem much further in time!

Multi-material treatment of high-order curvilinear zones: material indicator functions

- The remap phase generates mixed zones, where a **single computational element contains multiple material states**.
- Track materials with **material indicator functions**:

$$0 \leq \eta_k(x, t) \leq 1, \quad \sum_k \eta_k = 1, \quad \frac{d}{dt} \eta_k = 0$$

- ✓ discontinuous material characteristic functions are initially approximated with high-order fields
- ✓ the material indicators move with the mesh, so their dofs don't change in the Lagrangian phase

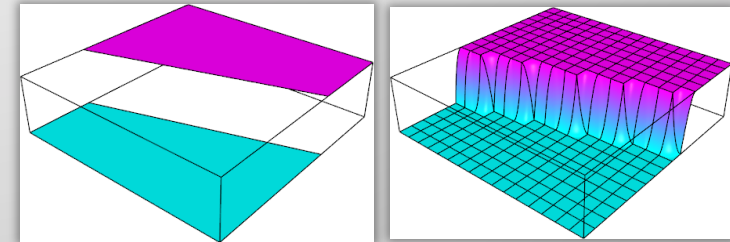
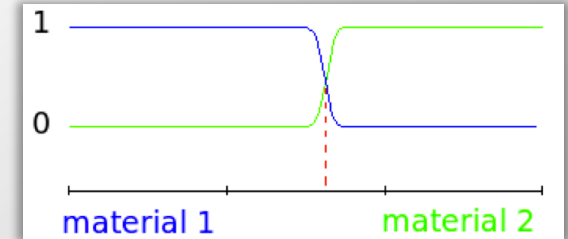
- Material-specific volume, mass, internal energy:

$$V_k = \int_{\Omega(t)} \eta_k, \quad M_k = \int_{\Omega(t)} \eta_k \rho, \quad IE_k = \int_{\Omega(t)} \eta_k \rho e$$

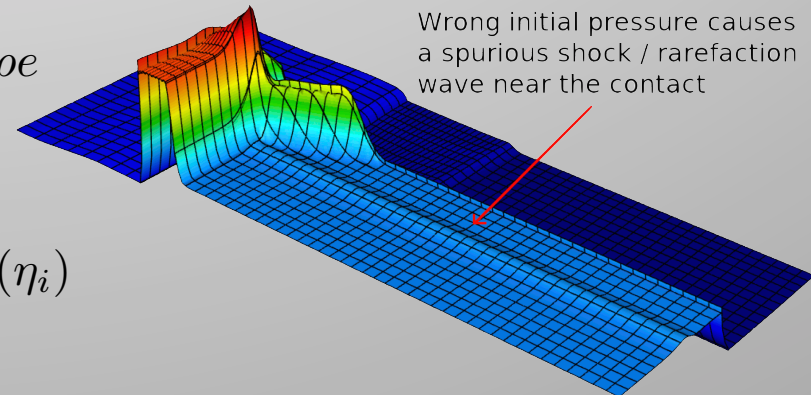
- Two pressure evaluation options:

$$p = \sum_k \eta_k p_k(\rho, e), \quad p = p_k(\rho, e), \quad k = \arg \max_i (\eta_i)$$

“material mixing” **“dominant material”**



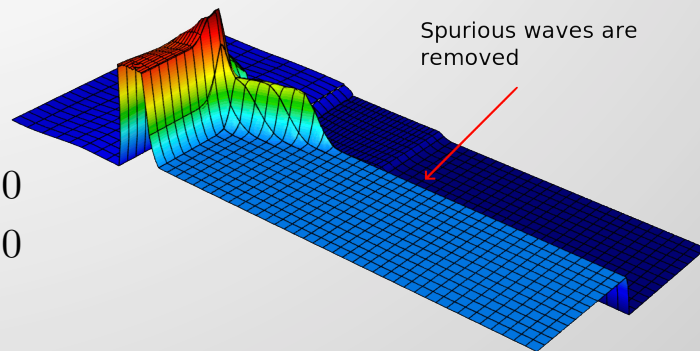
Simple material indicator function and its monotone projection with a Bernstein basis.



Multi-material treatment of high-order curvilinear zones: material-specific thermodynamic fields

To overcome the pressure initialization issue we break density and energy into material-specific parts:

$$\rho_k(x, 0) := \begin{cases} \rho(x, 0) & \eta_k > 0 \\ 0 & \eta_k = 0 \end{cases}, \quad e_k(x, 0) := \begin{cases} e(x, 0) & \eta_k > 0 \\ 0 & \eta_k = 0 \end{cases}$$



Material-specific mass and internal energy:

$$M_k = \int_{\Omega(t)} \eta_k \rho_k, \quad IE_k = \int_{\Omega(t)} \eta_k \rho_k e_k$$

Lagrangian density computation:

- ✓ $\{\rho_k\}$ evolved by strong mass conservation
- ✓ multi-material density $\rho = \sum_k \eta_k \rho_k$

Lagrangian internal energy computation:

- ✓ material-specific mass matrix, stress and corner forces
- ✓ by SMC \mathbf{M}_v and $\{\mathbf{M}_e^k\}$ do not change in time
- ✓ semi-discrete total energy conservation: $\mathbf{F} = \sum_k \mathbf{F}_k$

Single-material Lagrangian FEM

Momentum Conservation: $\mathbf{M}_v \frac{d\mathbf{v}}{dt} = -\mathbf{F} \cdot \mathbf{1}$

Energy Conservation: $\mathbf{M}_e \frac{de}{dt} = \mathbf{F}^T \cdot \mathbf{v}$

Equation of Motion: $\frac{d\mathbf{x}}{dt} = \mathbf{v}$

$$(\mathbf{M}_v)_{ij} = \int_{\Omega} \rho \vec{w}_i \cdot \vec{w}_j$$

$$(\mathbf{M}_e)_{ij} = \int_{\Omega} \rho \phi_i \phi_j$$

$$\mathbf{F}_{ij} = \int_{\Omega} (\sigma : \nabla \vec{w}_i) \phi_j$$

Multi-material Lagrangian FEM

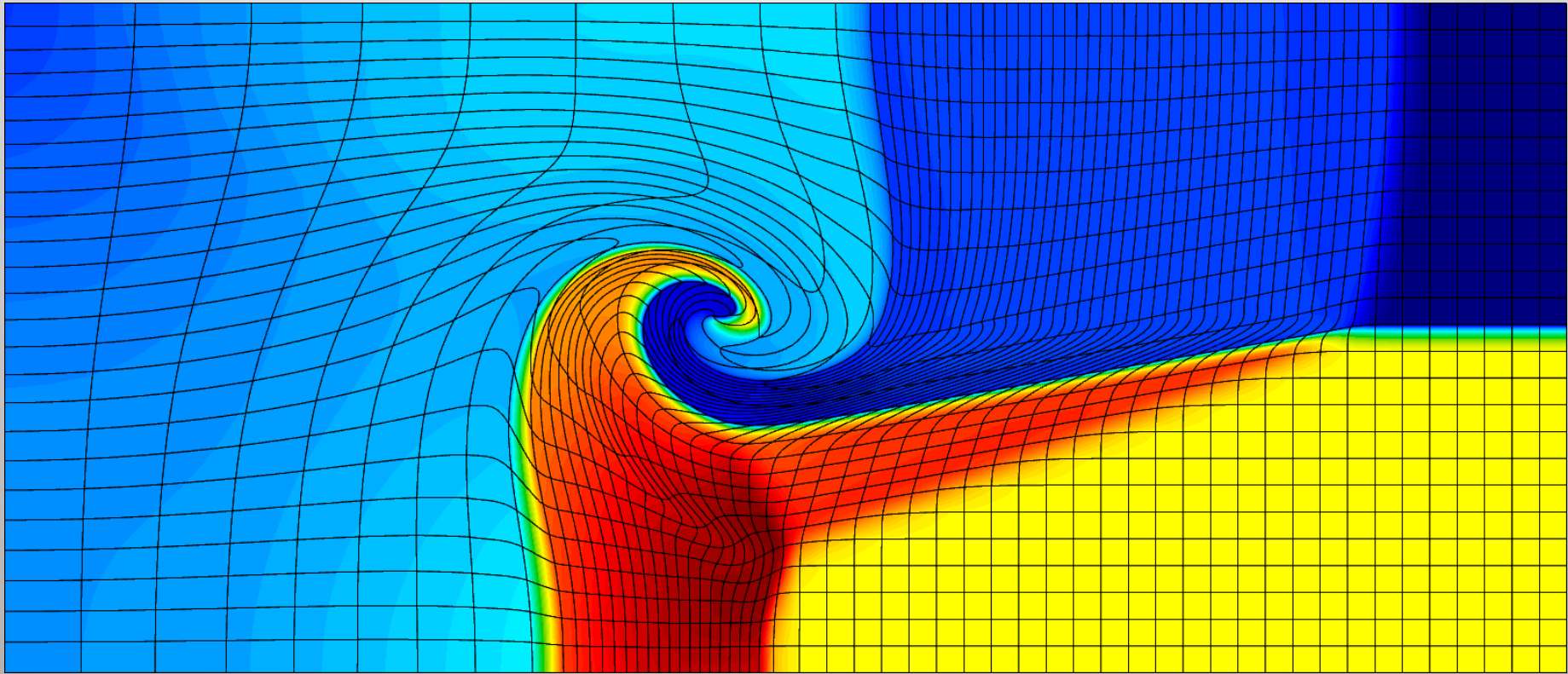
Momentum Conservation: $\mathbf{M}_v \frac{d\mathbf{v}}{dt} = -\mathbf{F} \cdot \mathbf{1}$

Energy Conservation: $\mathbf{M}_e^k \frac{de_k}{dt} = \mathbf{F}_k^T \cdot \mathbf{v}$

Equation of Motion: $\frac{d\mathbf{x}}{dt} = \mathbf{v}$

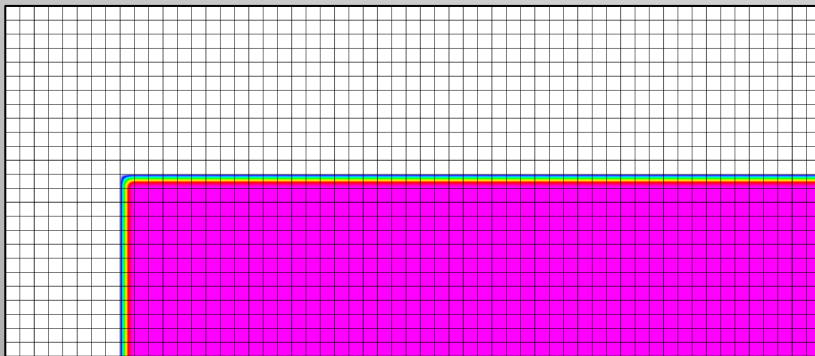
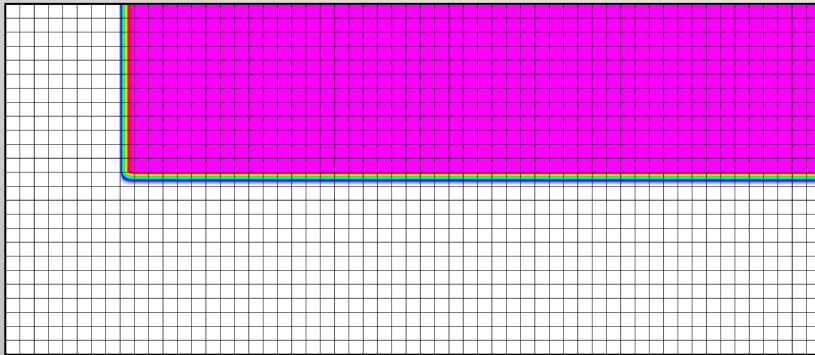
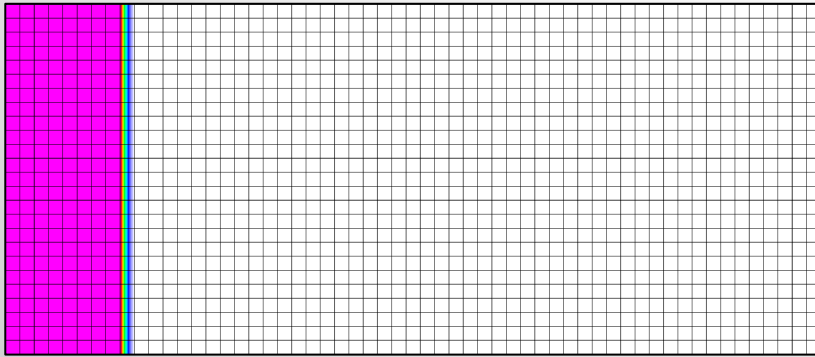
Lagrangian multi-material Triple-point – shock interaction in BLAST

- triple-point initialized at a center of a zone
- 3 material indicator functions
- Q3-Q2 method (positive Bernstein basis)
- material indicators use thermodynamic space

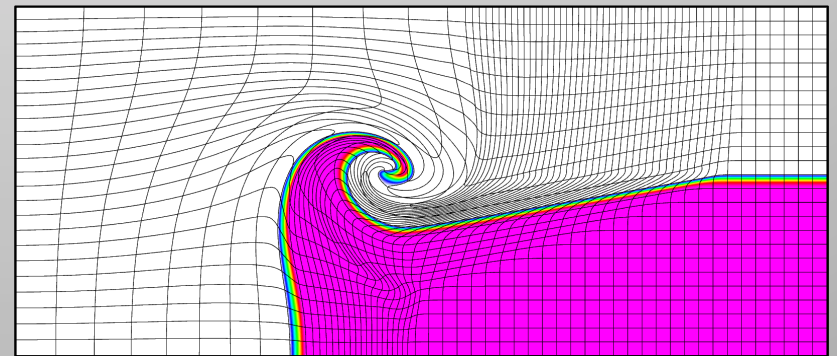
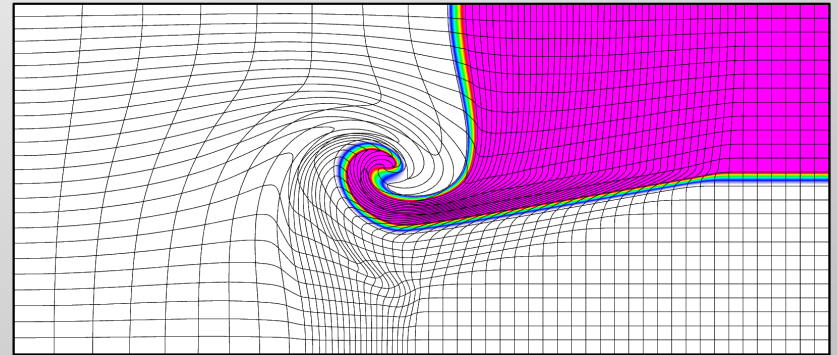
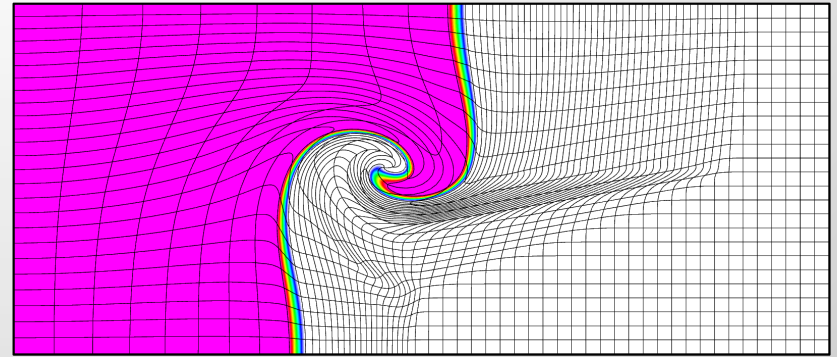


Multi-material density, $t=3$

Lagrangian multi-material Triple-point – shock interaction: evolution of material indicator functions

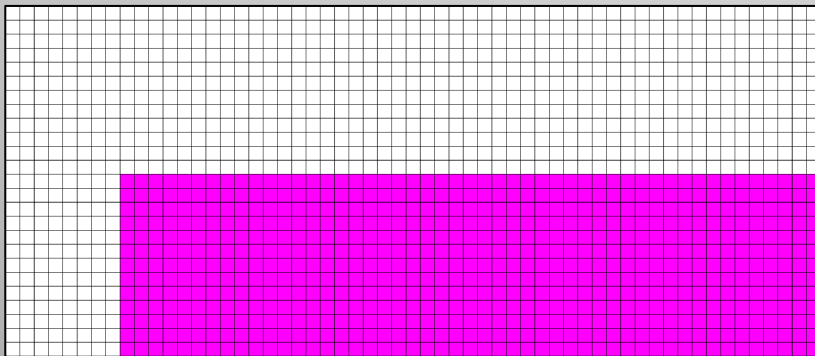
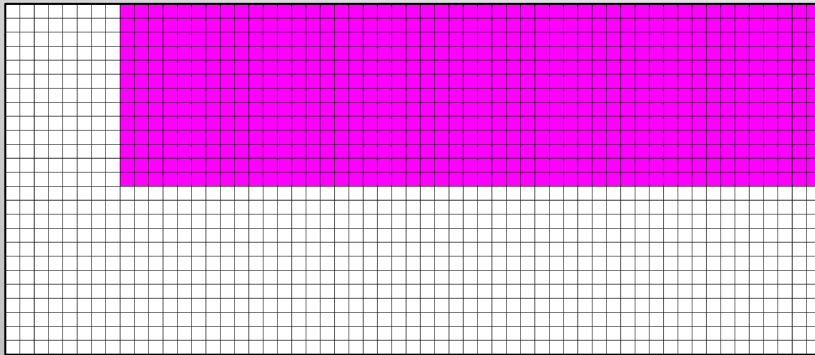
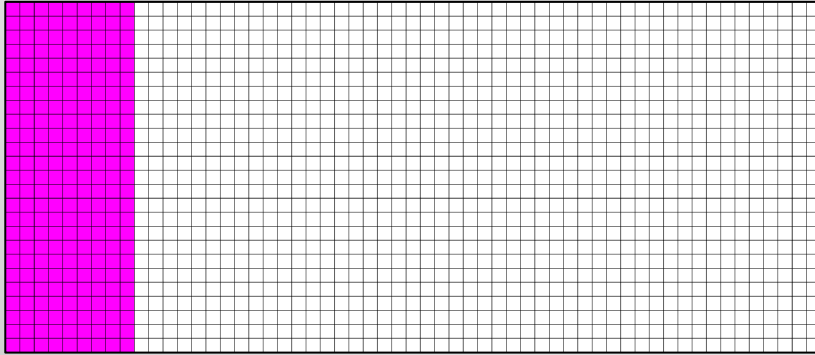


$t = 0$

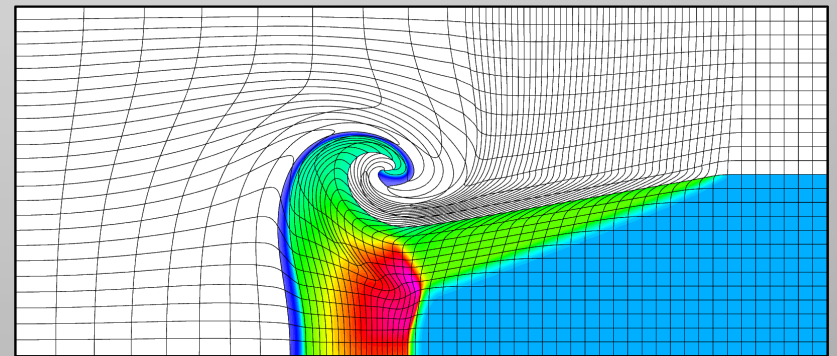
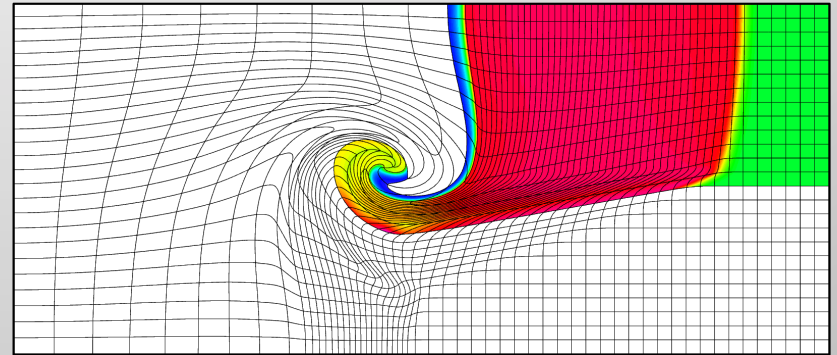
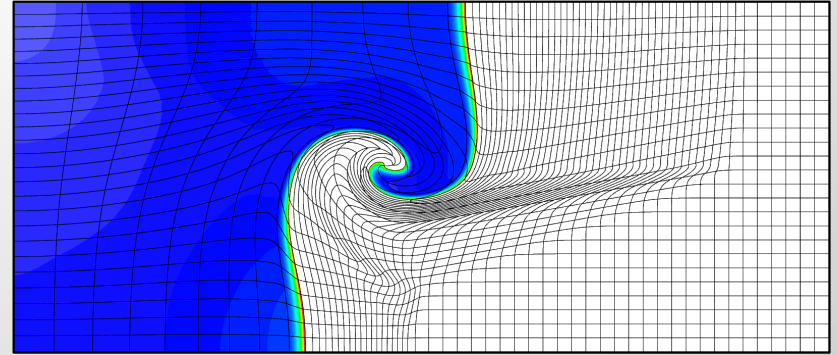


$t = 3$

Lagrangian multi-material Triple-point – shock interaction: evolution of material-specific densities



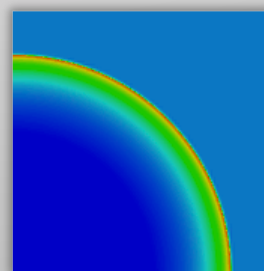
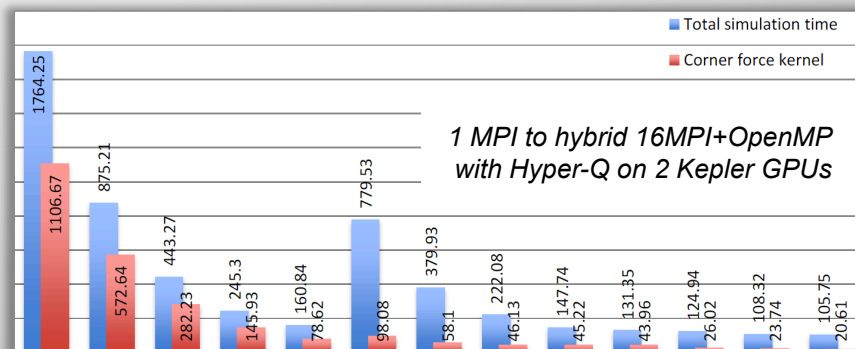
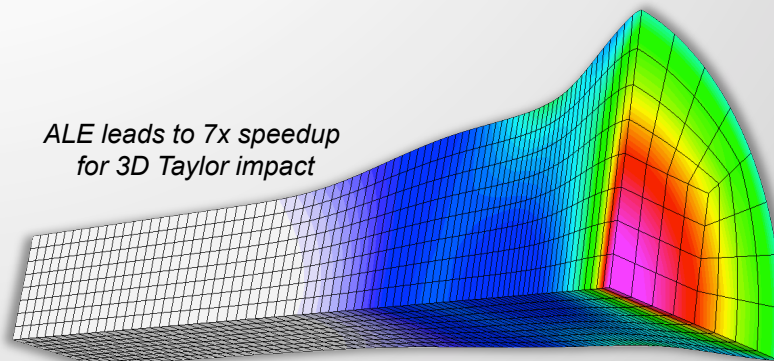
$t = 0$



$t = 3$

Current and future work

- Preliminary results with high-order ALE remesh+remap are promising
- Several approaches (LSD, FCT) seems to be effective for high-order monotonicity
- Initial Lagrangian multi-material results are encouraging
- More work is needed to:
 - improve monotonicity in BLAST
 - remap multi-material fields
- Some other recent research activities
 - Multi-resolution viscosity limiter for high-order hydrodynamics (**poster: T. Ellis**)
 - ALE remap for axisymmetric and elastic-plastic deformation problems (**poster: V. Dobrev**)
 - Large-scale parallel scalability and GPU/multi-core acceleration (**poster: V. Dobrev**)



Fourth order Sedov blast with multi-resolution limiter

